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UNCERTAINTY ANALYSIS FOR SECONDARY ENERGY DISTRIBUTIONS

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ABSTRACT

In many transport calculations the integral design parameter of interest (response) is determined mainly by secondary particles such as gamma rays from (n,γ) reactions or secondary neutrons from inelastic scattering events or (n,2n) reactions. Standard sensitivity analysis usually allows to calculate the sensitivities to the production cross sections of such secondaries, but an extended formalism is needed to also obtain the sensitivities to the energy distribution of the generated secondary particles. For a 30-group standard cross-section set 84% of all non-zero table positions pertain to the description of secondary energy distributions (SED's) and only 16% to the actual reaction cross sections. Therefore, any sensitivity/uncertainty analysis which does not consider the effects of SED's is incomplete and neglects most of the input data. This paper describes the methods of how sensitivity profiles for SED's are obtained and used to estimate the uncertainty of an integral response due to uncertainties in these SED's. The detailed theory is documented elsewhere and implemented in the LASL sensitivity code SENSIT. SED sensitivity profiles have proven particularly valuable in cross-section uncertainty analyses for fusion reactors. Even when the production cross sections for secondary neutrons were assumed to be without error, the uncertainties in the energy distribution of these secondaries produced appreciable uncertainties in the calculated tritium breeding rate. However, complete error files for SED's are presently nonexistent. Therefore, methods will be described that allow rough error estimates due to estimated SED uncertainties based on integral SED sensitivities.

As the number of cross-section sensitivity and uncertainty analyses (that are being performed for many specific design or research applications) increases, it is more and more realized that most of them are incomplete. In fact very often only the effects of uncertainties in total cross sections or some other conveniently defined composit cross sections (such as inelastic scattering or absorption cross sections) on integral design parameters (responses) are considered. However, even if the uncertainties of all partial cross sections for all materials used in the calculation were included in such studies - which is at present not possible because of the nonexistence of complete covariance data - the analysis would still be incomplete because the energy and angular distributions of secondaries from neutron reactions which produce secondary particles [e.g., (n,2n), (n,γ), inelastic scattering, etc.] are assumed to be without error. It is the goal of this paper to present a formalism which will allow the incorporation of uncertainties in secondary energy distributions into cross-section uncertainty analyses by using basically the same computational algorithms that are already available in existing analysis codes.

Figure 1 summarizes the classical formalism[1-3] which allows the calculation of an uncertainty in any computed integral response R due to uncertainties in any input parameters X_i which, in this context, are taken to be

RESPONSE $R = R(X_i)$

SENSITIVITY COEFFICIENT	SENSITIVITY PROFILE
$S_{X_i} = \dfrac{\partial R}{\partial X_i}$	$P_{X_i} = \dfrac{\partial R/R}{\partial X_i/X_i}$ (% per %)

ASSUMING LINEAR PERTURBATION THEORY
(small changes):

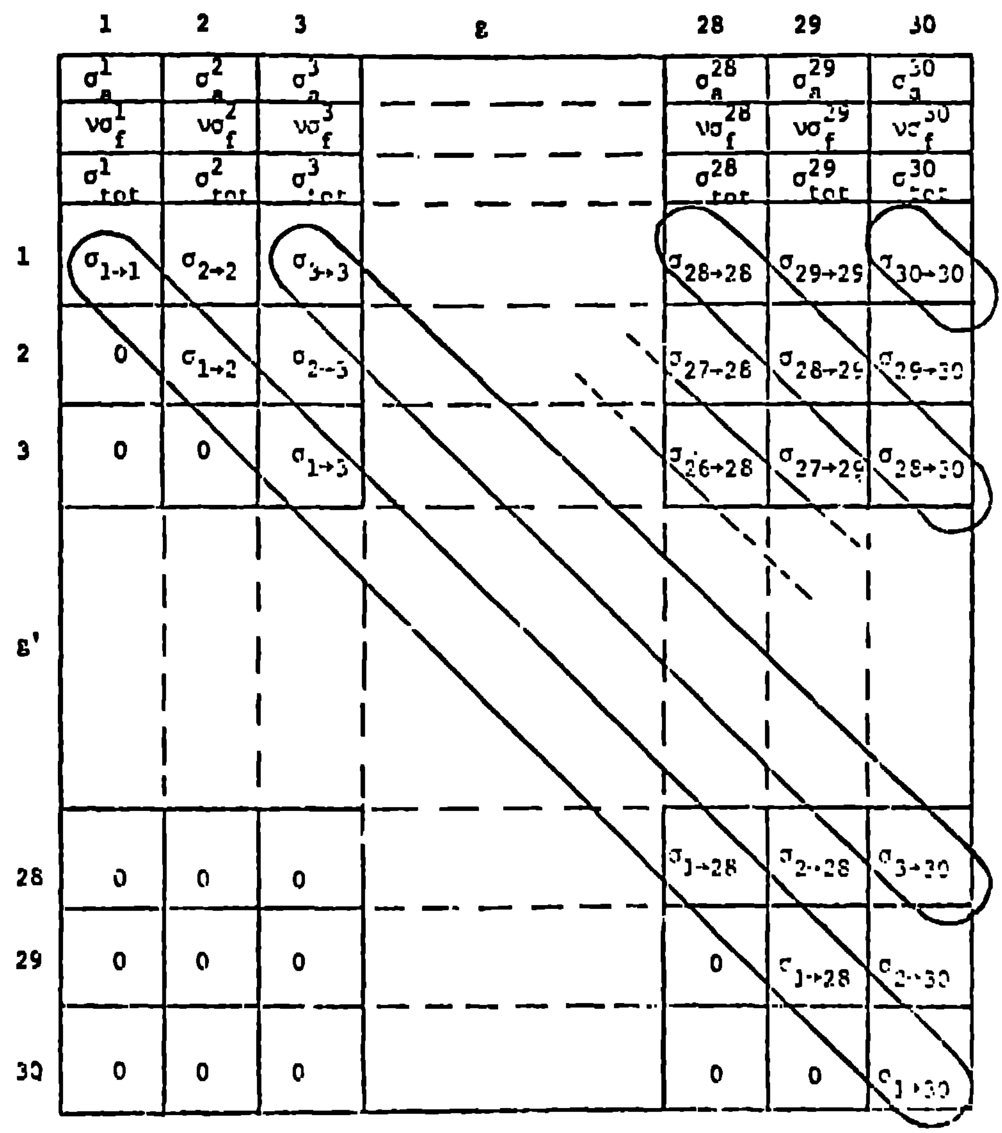
$\Delta R \approx S_{X_i} \cdot \Delta X_i$	$\dfrac{\Delta R}{R} \approx P_{X_i} \cdot \dfrac{\Delta X_i}{X_i}$

FOR DATA UNCERTAINTIES (δX_i) or $\mathrm{Cov}(X_i,X_j)$:

$\mathrm{Var}(R) = \sum_{i,j} S_{X_i} S_{X_j} \mathrm{Cov}(X_i,X_j)$	$\left(\dfrac{\Delta R}{R}\right)^2 = \sum_{i,j} P_{X_i} P_{X_j} \dfrac{\mathrm{Cov}(X_i,X_j)}{X_i X_j}$

Fig. 1. Summary of conventional sensitivity and uncertainty analysis methods.

input cross-section data, e.g., a multigroup cross-section set [illegible]. In order to use th[illegible] f[illegible]alism to incorporate uncertainties in secondary energy distributi[illegible]ED's), we must define appropriate sensitivity profiles and covaria[illegible]trices for SED's. Figure 2 shows the structure of a typical multigr[illegible]utron cross-section set (gamma rays are excluded for simplicity), w[illegible] those data which describe the SED's are encircled. Obviously, since fo[illegible] each incident neutron energy (index g') a whole



Total nonzero positions describing XS-set = 555

Total nonzero positions describing SED's = 465 (= 84% of total)

Fig. 2. Multigroup cross-section set for a 30 neutron-group structure, including only downscattering: [illegible]

spectrum of secondaries may be produced (index g), the two-dimensional array of the scattering matrix is needed to describe SED's. As a consequence, in the 30-group structure shown in Fig. 2, 84% of all cross-section data describe exclusively SED's. To convey some feeling for possible uncertainties in such SED data we reproduce in Fig. 3 a comparison of a recently measured secondary neutron energy spectrum[4] for $^9Be(n,2n)$ with data contained in ENDF/B-IV. Although these large discrepancies may be smoothed out after the data are converted into multigroup form, it appears nevertheless that the data uncertainties in SED's are considerable and should not be neglected. We shall return later to the question on how to quantify these uncertainties conveniently.

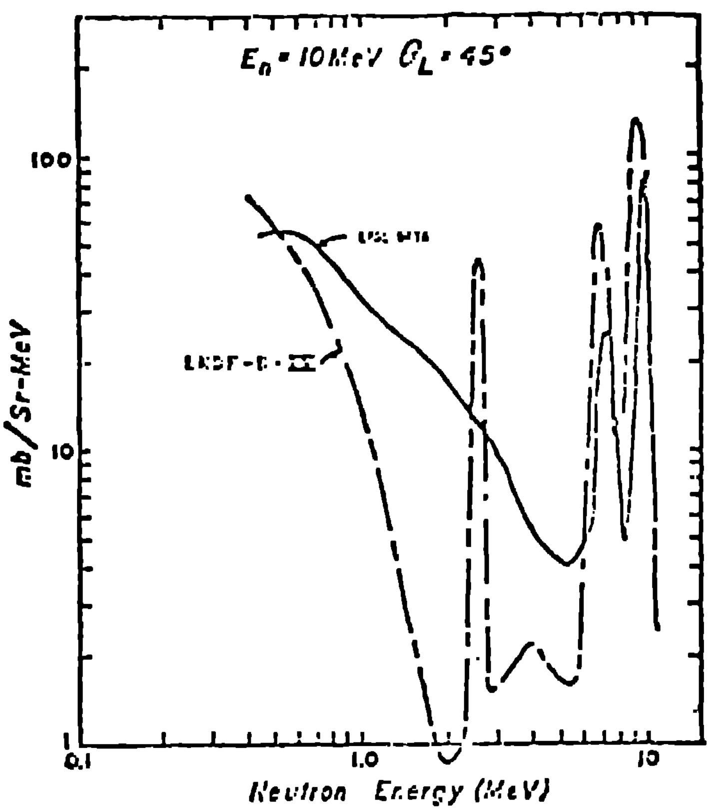


Fig. 3. Comparison of newly measured secondary energy distribution (smooth curve) with ENDF/B-IV data.

Fig. 4 gives a summary on how an analytical expression for the cross-section sensitivity profile P_{XS} can be derived[5] and shows at the same time that sensitivity profiles for SED's may be calculated from the adjoint expression of that for P_{XS}. The detailed analytical expression for an SED sensitivity profile[6] is shown in Fig. 5. Taking the incident neutron energy E' as a parameter and the emerging neutron energy E (energy of the secondary particle) as the continuous variable, we note that $P^{SED}_{\Sigma_{x,E'}}(E)$ spans again a two-dimensional array which means that in a multigroup representation one may expect one full SED sensitivity profile for each energy group specifying the incident neutron energy. From the expression in Fig. 5 it is obvious that P^{SED} can be physically interpreted in complete analogy to P_{XS} as the percentage change of the response R due to a one percent change in the value of $\Sigma_{g'\to g}$:

$$P^{SED}_{\Sigma_{x,g'}}(E_g) = \frac{\delta R/R}{\delta\Sigma_{g'\to g}/\Sigma_{g'\to g}} . \qquad (1)$$

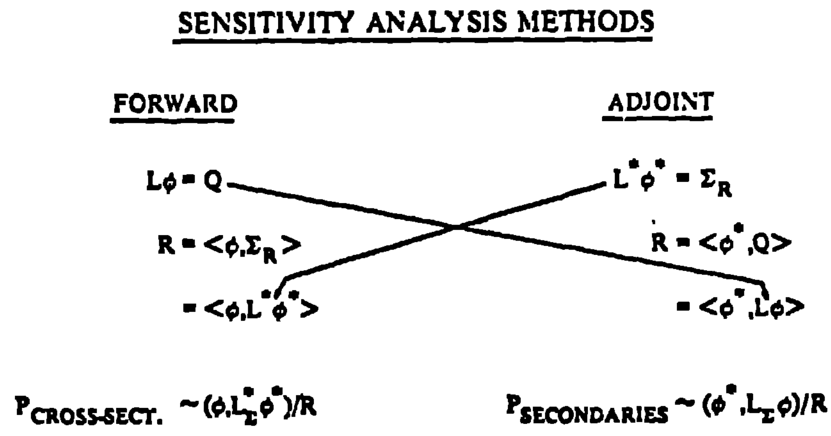


Fig. 4. Derivation of equations for cross-section and SED sensitivity profiles.

SENSITIVITY PROFILES FOR SECONDARY ENERGY (SED) AND ANGULAR (SAD) DISTRIBUTIONS

$$P^{SED}_{\Sigma^{E'}_x}(E) = \frac{1}{R}\int d^3r \int d^2\Omega \int d^2\Omega' \phi^*(r,E,\Omega)\Sigma_x(r;E'\rightarrow E,\Omega'\rightarrow\Omega)\phi(r,E',\Omega')$$

$$P^{SAD}_{\Sigma^{E'}_x}(\Omega) = \frac{1}{R}\int d^3r \int dE \int d^2\Omega' \phi^*(r,E,\Omega)\Sigma_x(r;E'\rightarrow E,\Omega'\rightarrow\Omega)\phi(r,E',\Omega')$$

Fig. 5. Detailed analytic expressions for SED and SAD sensitivity profiles.

One may also note that SED sensitivity profiles are always positive, i.e., they express "gain-terms" only. A specific example of two SED sensitivity profiles[6] is reproduced in Fig. 6, where also the associated secondary energy distributions $f_{2\rightarrow g}$ and $f_{3\rightarrow g}$ for incident energy groups 2 and 3 are shown with broken lines. The numbers above the top histogram indicate group numbers of our 30 energy group structure employed for this specific analysis.

The two-dimensionality of SED sensitivity profiles and of the secondary energy distribution itself often presents an obstacle when uncertainties of SED's are to be quantified in practice, especially when correlations are also considered. As a first step to quantify SED uncertainties, we introduce the concept of an integral SED uncertainty which can then be conveniently used for a comprehensive cross-section uncertainty analysis in connection with the definition of an integral SED sensitivity.[6] Figure 7 summarizes the definition of an integral SED sensitivity as introduced in Ref. 6. The basis for this definition is the fact that each secondary energy distribution itself may be subdivided into a "hot", i.e., high-energy part, and a "cold", i.e., low-energy part by identifying the median energy group g_m which is defined as that group into which the median energy of all secondaries (for a given initial neutron energy) falls. Then the associated SED sensitivity profile can be integrated separately over its cold part and its hot part. Subtracting these two integrals from each other, as indicated on Fig. 7, defines an integral SED sensitivity, S^{SED}, which may be labeled "HOT" if the difference is positive and "COLD" if it is negative. S^{SED} is then a quantitative measure of how much more sensitive the response R is to high-energy secondaries (if S^{SED} is "HOT") than to low-energy secondaries.

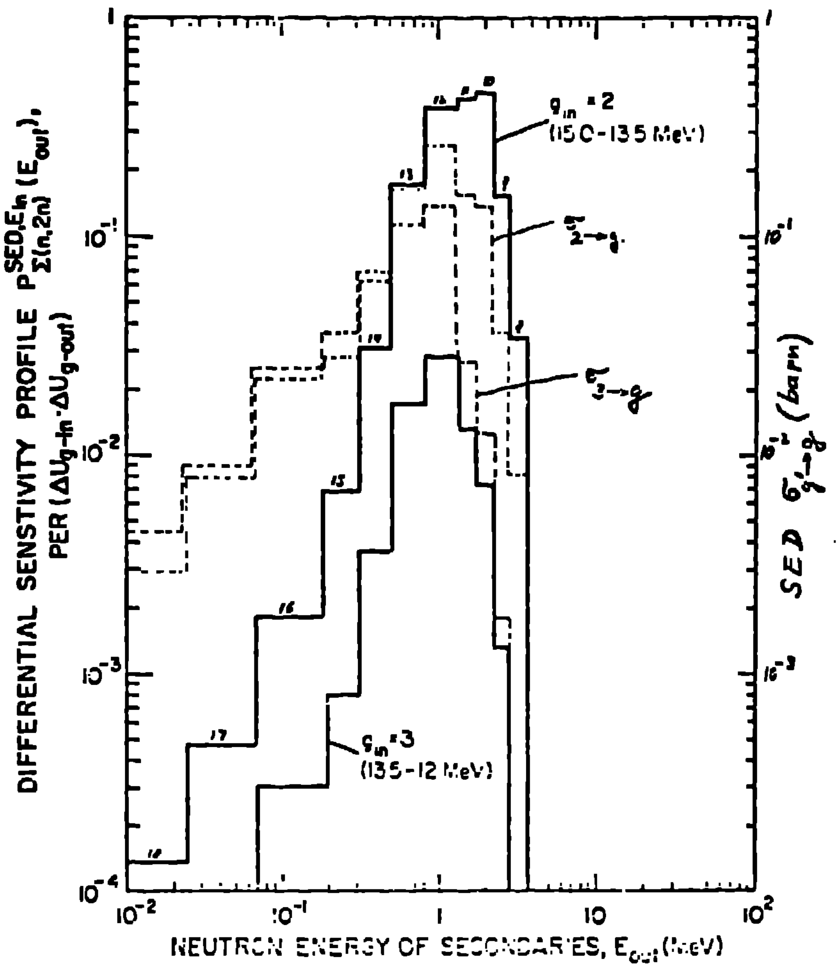


Fig. 6. Double-differential sensitivity profiles for the secondary energy distributions of Fe(n,2n) reactions for each energy group of initial neutrons, per lethargy widths of initial and final energy groups.

Since in general we have an SED for each incident energy group g', this definition of S^{SED} holds for all g'. If we abbreviate $P^{SED}_{\Sigma_{x,g'}}(E_g)$ with $P^{SED}_{g'g}$ we have

$$S^{SED}_{g'} = \sum_{g=1}^{g_m} P^{SED}_{g'g} - \sum_{g=g_m+1}^{G} P^{SED}_{g'g} \quad . \tag{2}$$

Within this concept it follows quite naturally then to also define an integral SED uncertainty as shown in Fig. 8. The spectral shape uncertainty parameter f may be considered as the width of an uncertainty band that can be drawn around an average secondary energy distribution which encompasses all credible data available for this particular SED. Consequently, if the number of hot secondaries is increased by a fraction

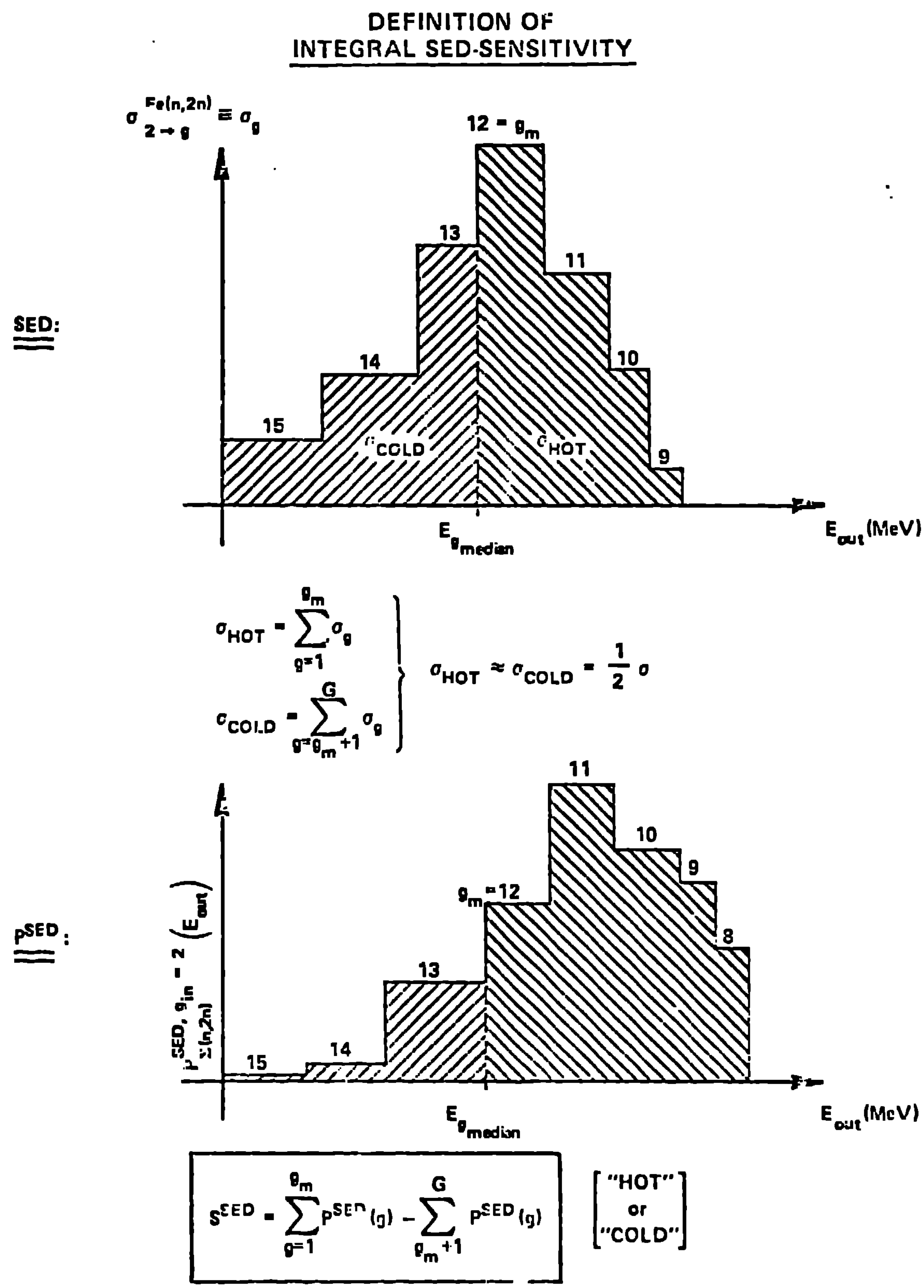
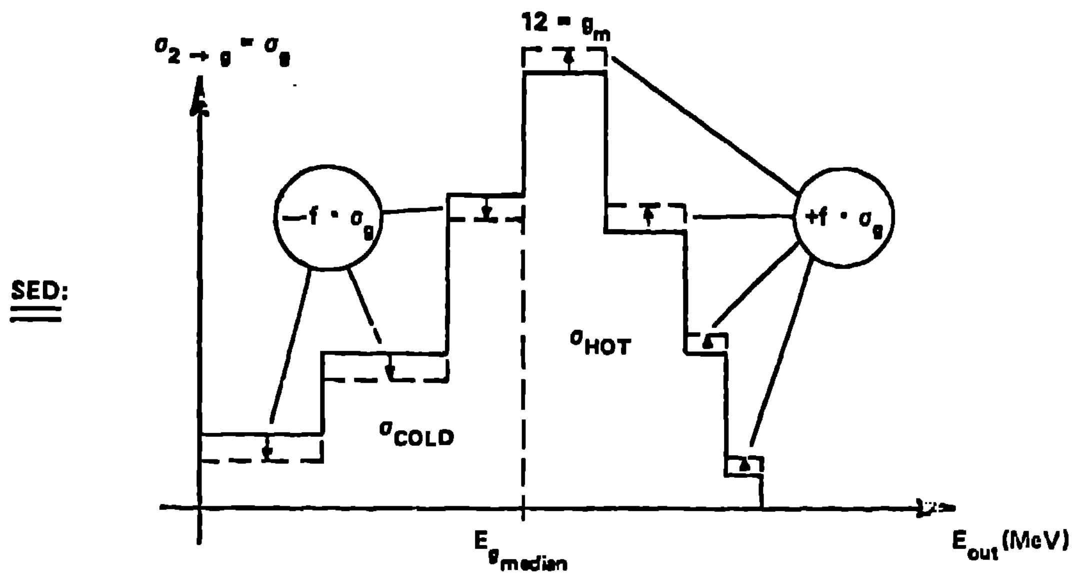


Fig. 7. Definition of median energy and integral SED sensitivity.

DEFINITION OF INTEGRAL SED-UNCERTAINTY "f" (SPECTRAL SHAPE UNCERTAINTY PARAMETER)



$$\frac{\delta\sigma_g}{\sigma_g} = \begin{cases} +f \text{ if } g \leq g_m \\ -f \text{ if } g > g_m \end{cases}$$

Fig. 8. Interpretation of integral SED uncertainty as spectrum shape perturbation.

f of all secondaries, while the number of cold secondaries is decreased by this same number, then f quantifies only the uncertainty in the shape of the SED while the total number of secondaries, i.e., the normalization of the SED remains unchanged. Thus f may also be interpreted as a measure for a spectrum shape perturbation which can be written as

$$\frac{\delta\sigma_{g'\to g}}{\sigma_{g'\to g}} = \begin{cases} +f_{g'}, \text{ if } g \leq g_m \\ -f_{g'}, \text{ if } g > g_m \end{cases} . \tag{3}$$

Returning for a moment to our original goal, namely to treat SED uncertainties within the same formalism than ordinary cross-section uncertainties (compare Fig. 1), we are attempting to propagate SED changes into a response change via an equation of the form

$$\left(\frac{\delta R}{R}\right)_{SED} = \sum_{g'g} P^{SED}_{g'g} \frac{\delta\sigma_{g'\to g}}{\sigma_{g'\to g}} . \tag{4}$$

if a spectrum perturbation $\delta F_{g'\to g}$ is considered. Inserting Eq. (3) into Eq. (4) and using Eq. (2) we obtain

$$\left(\frac{\delta R}{R}\right)_{SED} = \sum_{g'} S_{g'}^{SED} f_{g'} \quad , \tag{5}$$

which is exactly analog to the classic equation used to estimate the effects of a reaction cross-section perturbation on a response R. Continuing the exact analogy we can infer from Eq. (5) immediately the formalism required to treat correlated uncertainties. Let us denote with f_i the value of f for a specific nuclear reaction, e.g., (n,2n), at a specific incident neutron energy, e.g., $g_{in} = 2$, and let f_j correspond to some different reaction/energy combination, then the uncertainty in R due to correlated uncertainties of all SED's considered for one specific isotope is given by

$$\left(\frac{\Delta R}{R}\right)^2_{SED} \equiv \frac{\mathrm{Var}(R)}{R^2} = \sum_{i,j} S_i^{SED} S_j^{SED} \mathrm{Cov}(f_i, f_j) \quad . \tag{6}$$

An illustration of how the values of f may be obtained by an evaluator who has N independent measurements of the same SED available is shown in Fig. 9. Muir[7] has written a short FORTRAN program SPEC which performs these numerical operations on a set of input energy spectra.

FOR n=1,...,N INDEPENDENT MEASUREMENTS OF σ_g:

XS-EVALUATOR ASSIGNS WEIGHTS w_n, THEN

$$f^n = \frac{\sigma^n_{HOT} - \sigma^n_{COLD}}{\bar{\sigma}}, \quad \text{WHERE } \bar{f} = \sum_{n=1}^{N} w_n f_n = 0$$

$$\mathrm{Var}(f) = \overline{(f - \bar{f})^2} = \overline{f^2}$$

$$= \sum_{n=1}^{N} w_n \frac{\left(\sigma^n_{HOT} - \sigma^n_{COLD}\right)^2}{\bar{\sigma}^2}$$

Fig. 9. A sample evaluation of the spectral shape uncertainty parameter f.

Figure 10 summarizes the five steps necessary to perform a quantitative uncertainty analysis for SED's. The most difficult and time consuming part is listed as Step 3 which requires a cross-section evaluation to establish the numerical values for f_i. Our preliminary calculations and evaluations indicate that for a fusion reactor design problem (14 MeV neutron source) where the responses are taken to be total tritium production and nuclear heating, the integral SED sensitivities S_i range from 0.05 to 0.5 while the integral SED uncertainties f_i are of the order of 0.5 to 1.0.

In conclusion it should be noted that the methodology to include SED uncertainties into routine cross-section uncertainty analyses as

SED-UNCERTAINTY ANALYSIS (SUMMARY)

1) COMPUTE E_{median} OR g_m FOR ALL SED's

2) COMPUTE INTEGRAL SENSITIVITIES S^{SED}

$\boxed{\rightarrow \text{REQUIRES SENSITIVITY ANAL.}}$

3) OBTAIN SPECTRAL SHAPE PARAMETERS f_i FOR SED's

$\boxed{\rightarrow \text{REQUIRES XS-EVALUATION}}$

4) COMPUTE $Cov(f_i, f_j)$ FOR SPECIFIC REACTIONS AND SED's OF INTEREST

5) COMPUTE $\left(\frac{\Delta R}{R}\right)^2_{SED} = \sum_{i,j} S_i^{SED} S_j^{SED} Cov(f_i, f_j)$

Fig. 10. A five-step summary to perform SED uncertainty analysis.

presented here, requires a minimum of additional computations and allows rough estimates of spectral shape uncertainties to be considered quantitatively. If the correlations of the f_i's are unknown, certain conservative assumptions may be made to obtain at least an upper limit estimate for Var(R) as outlined in Ref. 3. If higher precision might be desired than the present model is able to give, an extension of the hot/cold subdivision of SED's appears straightforward to the point where individual energy groups may be considered. Also, it is clear that this formalism is not restricted in its application to secondary energy distributions but can be applied to quantify any spectral shape uncertainties, e.g., that of the fission spectrum.

REFERENCES

1. S. A. W. Gerstl, "The Application of Perturbation Methods to Shield and Blanket Design Sensitivity Analyses," AP/CTR/TM-28 or FRA/TM-67, Applied Physics Division, Argonne National Laboratory (1974).

2. D. E. Bartine, E. M. Oblow, and F. R. Mynatt, Nucl. Sci. Eng. 55, 147 (1974).

3. S. A. W. Gerstl, D. J. Dudziak, and D. W. Muir, "Cross-Section Sensitivity and Uncertainty Analysis with Application to a Fusion Reactor," Nucl. Sci. Eng. 26, 137-156 (1977).

4. D. M. Drake, G. F. Auchampaugh, E. D. Arthur, C. E. Ragan, and P. G. Young, "Double-Differential Beryllium Neutron Cross Sections at Incident Neutron Energies of 5.9, 10.1, and 14.2 MeV," Los Alamos Scientific Laboratory report LA-6257, August 1976.

5. S. A. W. Gerstl and W. M. Stacey, Jr., Nucl. Sci. Eng. 51, 339 (1973).

6. S. A. W. Gerstl, "Sensitivity Profiles for Secondary Energy and Angular Distributions," Proc. of the Fifth Int'l. Conf. on Reactor Shielding, Knoxville, Tenn., April 1977; R. W. Roussin, L. S. Abbott,

and D. E. Bartine (editors), Science Press, Princeton, USA, 1977 (pg. 101-111).

7. C. I. Baxman and P. G. Young (Eds.), "Applied Nuclear Data Research and Development, April 1-June 30, 1977," Los Alamos Scientific Laboratory report LA-6971-PR (1977).